10/538/13/ 10/936,134 YONG CHU 6-26-2006

\$%^STN; HighlightOn=; HighlightOff=;

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NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
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=> le reg

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=> file reg
COST IN U.S. DOLLARS

SINCE FILE TOTAL

FULL ESTIMATED COST ENTRY SESSION 0.21 0.21

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

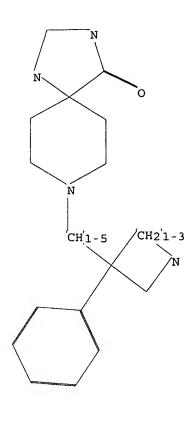
Please note that search-term pricing does apply when conducting SmartSELECT searches.

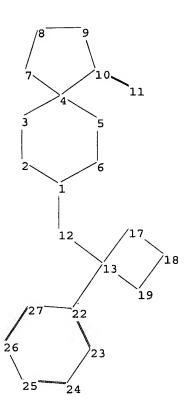
Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10936134\10936134.str





chain nodes : 11 12 ring nodes : 1 2 3 4 5 6 7 8 9 10 13 17 18 19 22 23 24 25 26 27 chain bonds : 1-12 10-11 12-13 13-22 ring bonds : $1-2^{-}$ 1-6 2-3 3-4 4-5 4-7 4-10 5-6 7-8 8-9 9-10 13-17 13-19 17-18 18-1922-23 22-27 23-24 24-25 25-26 26-27 exact/norm bonds : 1-2 1-6 1-12 2-3 3-4 4-5 4-7 4-10 5-6 7-8 8-9 9-10 10-11 13-17 13-19 17-18 18-19 exact bonds : 12-13 13-22 normalized bonds : 22-23 22-27 23-24 24-25 25-26 26-27

G1:X,Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:CLASS 12:CLASS 13:Atom 17:Atom 18:Atom 19:Atom 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom

L1 STRUCTURE UPLOADED

=> d L1 HAS NO ANSWERS L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 09:47:19 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED -

4 TO ITERATE

100.0% PROCESSED

4 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS:

200 4 TO

PROJECTED ANSWERS:

3 TO 163

L2

3 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 09:47:30 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 114 TO ITERATE

100.0% PROCESSED

114 ITERATIONS

66 ANSWERS

SEARCH TIME: 00.00.01

66 SEA SSS FUL L1

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COST IN U.S. DOLLARS

SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST

167.15 166.94

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=> s 13

6 L3 T.4

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Current appl.

L4 ANSWEP | OF 6 CAPLUS COPYRIGHT 2006 ACS ON STN ACCESSION NUMBER: 2004:534204 CAPLUS DOCUMENT NUMBER: 141:89006

DOCUMENT NUMBER: TITLE: IAI:89006
Preparation of pyrrolidine and azetidine compounds as CCR5 antagonists
Yang, Hanbiao: Kazmierski, Wieslaw Mieczyslaw;

INVENTOR(S): Aquino,

PATENT ASSIGNEE(S): SOURCE:

..

Christopher Joseph Smithkline Beecham Corporation, USA PCT Int. Appl., 130.pp. Glox. DOCUMENT TYPE: DOCUMENT TIPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION: English

	PATENT NO.						KIND DATE				APPL	ICAT						
	WO 2004055016				A1 20040701			,	WO 2	003-	20031212							
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			GE,	GH,	GM,	HR,	HU,	ID,	ĪL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,
			LK.	LR.	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,
			NZ.	OM,	PG,	PH,	PL,	PT,	RO,	RU,	sc,	SD,	SE,	SG,	SK,	SL,	SY,	TJ,
			TM.	TN.	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	vc,	VN,	Yυ,	ZA,	ZM,	ZW	
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OTHER SOURCE(S): MARPAT 141:89006

ARISMER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN 716326-99-1p 716326-70-4p 716326-71-5p 716326-72-6p 716326-73-7p 716326-74-8p 716326-73-p 716326-74-8p 716326-75-pp 716326-76-0p 716326-77-1p 716326-82-p 716326-82-p 716326-80-6p 716326-80-6p 716326-80-6p 716326-80-6p 716326-80-7p 716326-91-2p 716326-93-3p 716326-96-p7 716326-97-5p 716326-93-6p 716326-97-5p 716327-01-4p 716327-05-8p 716327-05-p7 716327-05-p7 716327-05-p7 716327-05-p7 716327-05-p7 716327-05-p7 716327-05-p7 716327-05-p7 716327-05-p7 716327-13-8p 716327-12-p7 716327-13-8p 716327-12-p7 716327-13-p7 716327-22-pp 716327-21-p7 716327-22-pp 716327-22-pp

Therapeutic use; BIOL (Biological study); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)

(19repn. of pyrrolidine and azetidine derivs. as CCRS antagonists)

RN 716326-63-5 CAPLUS

(N 1-Pyrolidinecetrboxylic acid.

3-(3,-dichlorophenyl)-3-(3-(4-oxo-1-phenyl1,3,8-triazaspiro[4.5]dec-8-yl)propyl]-, 1,1-dimethylethyl ester (9CI)

(CA INDEX NAME)

716326-64-6 CAPLUS
Pyrrolidine, 3-(3,4-dichlorophenyl)-1-(2-furanylcarbonyl)-3-(3-(4-oxo-1-pheny)-1,3,6-triazaspiro[4.5]dec-8-yl)propyl)- (9CI) (CA INDEX NAME)

7]6326-65-7 CAPLUS
Pyrrolidine, 3-(3,4-dichlorophenyl)-1-(2-furanylcarbonyl)-3-[3-(4-oxo-1-phenyl-1,3,8-triazaspiro[4.5)dec-8-yl)propyl]-, mono(trifluoroacetate)
(9C1) (CA INDEX NAME)

14 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

$$R^3 - (Y)_m - B = X - A - (R^2)_m$$

Title compds. I [R1 = (un)substituted-alkyl, -alkynyl, -cycloalkyl, -heterocyclyl, etc., or R1 and X taken together form a saturated,

partially
saturated or aromatic 5-6 membered ring having 0-3 heteroatoms selected
from O.
P, S, or N that is fused to ring A/ R2 - OH, halogen (un)substitutedalkyl, -alkoxy, -aryl, -heteroaryl, -cycloalkyl, etc., or two geminal R2s
are optionally taken together to from a spiro, saturated, partially
saturated or
aromatic 5-6 membered ring having 0-3 heteroatoms selected from O, P, S,

N, said fused or spiro ring optionally substituted; R3 = H, halo, cyano, trifluoromethyl, (un)substituted amino, acylamino, alkyl; R9 = H or oxo;

= Ci-5 alkylene, optionally substituted with oxo, thioxo, -S(O)t where τ

l or 2, halogen atoms, or alkyl and optionally containing 1-3 oxygen, nitrogen, sulfur, or phosphorus atoms: Y = carbonyl, thiocarbonyl, 1,2-dioxocethylene, alkyl, alkenyl, etc.: A = saturated, partially saturated, or aromatic 3-7 monocyclic or 8-10 membered bicyclic ring having one ring nitrogen and 0-4 addnl. heteroatoms selected from 0, P, Sor N; m = 0 or 1, n = 0-5;] and their pharmaceutically acceptable salts are prepared and disclosed as CCRS antagonists. Thus, II was prepared via condensation of tert-Bu 3-(3,4-dichlorophenyl)-3-(3-oxopropyl)pyrrolidne-1-carboxylate (preparation given) with the amine III followed by deprotection and acylation
with 2-furanoyl chloride. I have nicks with a single parameters.

ation with 2-furancyl chloride. I have pICSO values of ≥5 in assays for CCR5 antagonism. As CCR5 antagonists, I are useful for the treatment of viral infections (particularly HIV infection). 716326-63-57 16326-64-69 716326-65-79 716326-68-89 716326-67-99 716326-68-09

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

1

CRN 716326-64-6 CMF C31 H34 C12 N4 O3

CRN 76-05-1 CMF C2 H F3 O2

RN 716326-66-8 CAPLUS
CN Pyrrolidine,
3-{3,4-dichlorophenyl}-1-{5-isoxatolylcarbonyl}-3-{3-{4-oxo-1-phenyl-1,3,8-triazaspiro{4,5}dec-8-yl}propyl}- (9C1) (CA INDEX NAME)

CM 1

CRN 716326-66-8

2

CRN 76-05-1 CMF C2 H F3 O2

716326-68-0 CAPLUS
Pyrrolidine, 3-(3,4-dichlorophenyl)-3-[3-(4-oxo-1-phenyl-1,3,8-triazaspiro(4-5)dec-8-yl)propyl]-1-(1H-pyrrol-2-ylcarbonyl)- (9CI) (CA INDEX NAME)

716326-69-1 CAPLUS
Pytrolidine, 3-{3,4-dichlorophenyl}-3-[3-(4-oxo-1-phenyl-1,3,8-triazaspirc(4.5)dec-8-yl)propyl]-1-{1H-pytrol-2-ylcarbonyl}-,
monottrifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 716326-68-0 CMF C31 H35 C12 N5 O2

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

RN 716326-72-6 CAPLUS
CN Pyrrolidine.
3-(3,4-dichlorophenyl)-1-(2-furanylcarbonyl)-3-[3-[4-oxo-1-[3-(trifluoromethyl)phenyl]-1,3,8-triazaspiro(4.5)dec-8-yl]propyl]-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 716326-71-5 CMF C32 H33 C12 F3 N4 O3

2 CM

CRN 76-05-1 CMF C2 H F3 02

716326-73-7 CAPLUS
Pyrrolidine, 1-(cyclobutylcarbonyl)-3-(3,4-dichlorophenyl)-3-(3-[4-oxo-1-]3-(t)riluoromethyl)phenyl}-1,3,8-triazaspiro[4.5]dec-8-ylpropyl]- (9CI)
(CA INDEX NAME)

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

716326-70-4 CAPLUS
Pyrrolidine, 3-{3,4-dichlorophenyl}-1-(1-oxopentyl)-3-{3-[4-oxo-1-[3-(trifluoromethyl)phenyl}-1,3,8-triazaspiro[4.5]dec-8-yl]propyl]- (9CI)

RN 716326-71-5 CAPLUS
CN Pyrrolidine.
1(3,4-dichlorophenyl)-1-(2-furanylcarbonyl)-3-[3-[4-oxo-1-[3-(trifluoromethyl)phenyl]-1,3,8-triazaspiro[4.5]dec-8-yl]propyl]- (9CI)
(CA INDEX NAME)

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

716326-74-8 CAPLUS
Pyrrolidine, l-(cyclobutylcarbonyl)-3-(3,4-dichlorophenyl)-3-[3-[4-oxo-1-[3-(trifluoromethyl)phenyl]-1,3,8-triazaspiro[4.5]dec-8-yl]propyl]-,
mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 716326-73-7 CMF C32 H37 C12 F3 N4 O2

$$c_1 = c_1 = c_1$$

2

CRN 76-05-1 CMF C2 H F3 02

716326-75-9 CAPLUS
Pytrolldine, 3-(3,4-dichlorophenyl)-1-(1-oxopentyl)-3-(3-(4-oxo-1-phenyl-1,3,8-triezaspiro(4.5)dec-8-yl)propyl]- (9C1) (CA INDEX NAME)

RN 716326-76-0 CAPLUS
CN Pyrrolidine,
1-tcyclopentylcarbonyl)-3-{3,4-dichlorophenyl}-3-{3-(4-oxo-1-phenyl-1,3,8-triazaspiro[4,5]dec-8-yl)propyl}- (9CI) (CA INDEX NAME)

716326-77-1 CAPLUS
Pyrrolidine, l-(cyclobutylcarbonyl)-3-(3,4-dichlorophenyl)-3-[3-(4-oxo-1-phenyl-1,3,8-triazaspiro[4.5]dec-8-yl)propyl]- (9CI) (CA INDEX NAME)

716326-78-2 CAPLUS
Pyrrollding, I-(cyclobutylcarbonyl)-3-(3,4-dichlorophenyl)-3-(3-(4-oxo-1-phenyl-1,3,8-triazaspiro[4,5]dec-8-yl)propyl]-, mono(trifluoroacetate)
19C11 (CA INDEX NAME)

CM I

CRN 716326-77-1 CMF C31 H38 C12 N4 O2

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

CM 2

CRN 76-05-1 CMF C2 H F3 O2

716326-81-7 CAPLUS
1.3,8-Triazaspiro[4.5]decan-4-one, 3-acetyl-8-[3-[1-acetyl-3-(3,4-dichlorophenyl)-3-pyrrolidinyl]propyl]-1-(3-methylphenyl)- (9CI) (CA INDEX NAME)

716326-82-8 CAPLUS
1,3,8-Triazaspiro[4.5]decan-4-one, 3-acetyl-8-[3-[1-acetyl-3-[3,4-dichlorophenyl]-3-pyrrolidinyl]propyl}-1-[3-methylphenyl]-,
mono(trifluoroacetate) [9CI] (CA INDEX NAME)

CM L

CRN 716326-81-7 CMF C31 H38 C12 N4 O3

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

2 СМ

CRN 76-05-1 CMF C2 H F3 O2

716326-79-3 CAPLUS
Pyrrolidine, 1-(cyclobutylcarbonyl)-3-(3,4-dichlorophenyl)-3-(3-[1-(3-methylphenyl)-4-oxo-1,3,8-triazaspiro[4.5]dec-8-yl]propyl}- (9CI) (CA INDEX NAME)

716326-80-6 CAPLUS
Pyrrolidine, 1-(eyclobutylcarbonyl)-3-(3,4-dichlorophenyl)-3-[3-[1-(3-methylphenyl)-4-oxo-1,3,8-triazaspiro[4,5]dec-8-yl]propyl]-,
monottrifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 716326-79-3 CMF C32 H40 C12 N4 O2

L4 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

2

CRN 76-05-1 CMF C2 H F3 O2

716326-83-9 CAPLUS
1,3,8-Triazaspiro[4.5]decan-4-one, 8-[3-[1-(2-benzoxazoly1)-3-(3,4-dichloropheny1)-3-pyrrolidiny1)propy1)-1-pheny1- (9CI) (CA INDEX NAME)

716326-84-0 CAPLUS
1,3.8-Triazaspiro[4.5]decan-4-one, 8-[3-[1-(2-benzoxazolyl)-3-(3,4-dichlorophenyl)-3-pyrrolidinyl]propyl]-1-phenyl-, mono(trifluoroscetata)
(SCI) (CA INDEX NAME)

CM 1

CRN 716326-83-9 CMF C33 H35 C12 N5 O2

СМ 2

CRN 76-05-1 CMF C2 H F3 O2

716326-94-2 CAPLUS
Azetidine, 3-(3,4-dichlorophenyl)-3-[3-(4-oxo-1-phenyl-1,3,8-triazaspiro(4.5)dec-8-yl)propyl]-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

RN 716326-95-3 CAPLUS
CN Formic acid, compd. with
3-(3,4-dichlotophenyl)-3-{3-(4-oxo-l-phenyl-1,3,8triaxaspiro(4.5)dec-8-yl)propyl]-1-(phenylsulfonyl)azetidine (1:1) (9CI)
(CA INDEX NAME)

CM 1

CRN 716326-94-2 CMF C31 H34 C12 N4 O3 S

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
Pyrrolidine, 3-(3,4-dichlorophenyl)-1-(2-furanylcarbonyl)-3-(2-(4-oxo-1-phenyl-1,3,8-triazaspiro[4.5]dec-8-yl)ethyl]- (9CI) (CA INDEX NAME)

716326-99-7 CAPLUS
Pyrrolidine, 3-(3,4-dichlorophenyl)-3-[3-(4-oxo-1-phenyl-1,3,8-triazaspiro(4.5]dec-8-yl)propyl]-1-(1H-pyrazol-4-ylcarbonyl)- (9CI) (CA (NDEX NAME)

716327-00-3 CAPLUS
Pyrrolidine, 3-(3,4-dichlorophenyl)-1-[[5-(1,1-dimethylethyl)-2-turanyl]carbonyl]-3-[3-(4-oxo-1-phenyl-1,3,8-triazaspiro[4.5]dec-8-yl)propyl)- (9CI) (CA INDEX NAME)

716327-01-4 CAPLUS
1,3,8-Triazaspro[4.5]decan-4-one, 8-[3-[3-{3,4-dichloropheny1}]-1-(4,5-dihydro-1+-imidazol-2-y1)-3-pyrrolidiny1]propy1]-1-pheny1- (9CI) (CA INDEX NAME)

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

2

64-18-6 C H2 O2

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716326-96-4 CAPLUS
Azetidine, 3-[3,4-dichlorophenyl]-1-(2-furanylcarbonyl)-3-[3-(4-oxo-i-phenyl-1,3,8-triazaspiro[4.5]dec-8-yl)propyl]- (9C1) (CA INDEX NAME)

716326-97-5 CAPLUS
Azetidine, 1-(cyclopentylcarbonyl)-3-(3,4-dichlorophenyl)-3-(3-(4-oxo-l-phenyl-1,3,8-triazapiro[4.5)dec-8-yl)propyl)- (9CI) (CA INDEX NAME)

716326-98-6 CAPLUS

(Continued) ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

716327-02-5 CAPLUS
1-Pyrrolidinecarboxylic acid, 3-(3,4-dichlorophenyl)-3-[3-{1-(3-methylphenyl)-4-oxo-1,3,8-triszaspiro[4.5]dec-8-yl]propyl}-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

716327-03-6 CAPLUS
1-Pyrrolidinecarboxylic acid, 3-(3,4-dichlorophenyl)-3-(3-{1-(3-methoxyphenyl)-4-oxo-1,3,8-triazaspiro(4.5]dec-8-yl]propyl]-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

716327-04-7 CAPLUS
1-Pyrrolidinecerboxylic acid, 3-(3,4-dichlorophenyl)-3-[3-[4-oxo-1-[4-trifluoromethyl)phenyl]-1,3,8-triazaspiro[4.5]dec-8-yl]propyl}-,
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

716327-05-6 CAPLUS
1.3,6-Triazaspiro[4.5]decan-4-one, 8-[3-[1-(2-benzothiazoly1)-3-(3,4-dichloropheny1)-3-pyrrolidiny1)propy1]-1-pheny1- (9CI) (CA INDEX NAME)

716327-06-9 CAPLUS
1,3,8-Triazaspiro[4.5]decan-4-one, 8-[3-[1-(1H-benzimidazol-2-yl)-3-(3,4-dichlorophenyl)-3-pyrrolidinyl]propyl]-1-phenyl- (9CI) (CA INDEX NAME)

716327-07-0 CAPLUS
Pyrrolidine, 3-3(3-dichlorophenyl)-3-[3-(1-(3-methylphenyl)-4-oxo-1,3,8-tiazaspiro[4.5]dec-8-yllpropyl]-1-(1-oxopentyl)- [9C1) (CA INDEX NAME)

ANSWER I OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

7[63:7-1]-6 CAPLUS
1, 3, 8-friazaspiro[4.5]decan-4-one, 3-(cyclobutylcarbonyl)-8-[3-[1-(cyclobutylcarbonyl)-3-(3, 4-dichlocophenyl)-3-pyrrolidinyl|propyl)-1-[3-trifluoromethyl)phenyl]- (9Cl) (CA INDEX NAME)

716327-12-7 CAPLUS

716327-13-8 CAPLUS
Pyrrolidine, 1-(cyclopentylcarbonyl)-3-(3,4-dichlorophenyl)-3-[3-[1-(3-methoxyphenyl)-4-oxo-1,3,8-triazaapiro[4.5]dec-8-yl)propyl]- (9CI) (CA (NDEX NAME)

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

716327-08-1 CAPLUS
Pyrrolidine, 1-(cyclobutylcarbonyl)-3-(3,4-dichlorophenyl)-3-[3-[1-{3-mathoxyphenyl)-4-oxo-1,3,8-triazaspiro[4.5]dec-8-yl]propyl}- (9CI) (CA INDEX NAME)

716327-09-2 CAPLUS

RN 16327-09-2 CAFADO
CN Pyrrolidine,
3-(3,4-dichlorophenyl)-3-[3-[1-(3-methoxyphenyl)-4-oxo-1,3,8triezaspiro[4.5]dec-8-yl]propyl]-1-(1-oxopentyl)- (9CI) (CA INDEX NAME)

716327-10-5 CAPLUS
Pyrrolidine, 3-{3,4-dichlorophenyl}-1-{5-isoxazolylcarbonyl}-3-{3-{1-(3-methoxyphenyl})-4-oxo-1,3,8-triazaspiro{4.5}dec-8-yl}propyl}- (9CI) (CA INDEX NAME)

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 716327-14-9 CAPLUS
CN 1-Pyrrolidinecarboximidic acid,
N-cyano-3-(3,4-dichlorophenyl)-3-[3-[1-(3-methylphenyl)+d-oxo-1,3,8-triazaspiro[4.5]dec-8-yl]propyl]-, phenyl ester
(9CI) (CA INDEX NAME)

716327-15-0 CAPLUS
Pyrrolidine, l-(cyclopentylcarbonyl)-3-(3,4-dichlorophenyl)-3-[3-{1-(3-methylphenyl)-4-oxo-1,3,8-triataspiro[4.5}dec-8-yl]propyl)- (9CI) (CA INDEX MAME)

CAPLUS

1.3,8-Triazaspiro[4.5]decan-4-one, 3-(cyclopentylcarbonyl)-8-[3-{l-(cyclopentylcarbonyl)-3-(3,4-dichlorophenyl)-3-pyrrolidinyl]propyl}-1-(3-methylphenyl)- (9CI) (CA INDEX NAME)

716327-17-2 CAPLUS
1,3,8-Triazaspiro[4.5]decan-4-one, 3-(cyclobutylcarbonyl)-8-[3-[1-(cyclobutylcarbonyl)-3-(3,4-dichlorophenyl)-3-pyrrolidinyl)propyl}-1-(3-mathylphenyl)- |9c1| (CA INDEX NAME)

716327-18-3 CAPLUS
Pyrrolidine, 3-(4-chlorophenyl)-1-(cyclobutylcarbonyl)-3-[3-[4-oxo-1-{3-(trifluoromethyl)phenyl]-1,3,6-triezaspiro[4.5]dec-8-yl]propyl]- (9CI)
(CA INDEX NAME)

716327-19-4 CAPLUS
1.3.8-Triazaspiro(4.5)decan-4-one, 8-[3-[3-(3,4-dichlorophenyl)-1-(1-oxopentyl)-3-pyrrolidinyl)propyl|-3-(1-oxopentyl)-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

7|6328-43-7 CAPLUS
Pyrrolidine, 1-acetyl-3-(3,4-dichlorophenyl)-3-(3-(1-(3-methylphenyl)-4-oxo-[3,8-triazaspiro[4,5]dec-8-yl]propyl]- (9CI) (CA INDEX NAME)

REFERENCE COUNT: 3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 716327-20-7 CAPLUS
CN 1-Pyrrolidinecarboxylic acid,
3-(3,4-dichlorophenyl)-3-[3-(4-oxo-1-phenyl1,3,8-triazaspiro[4.5]dec-8-yl)propyl]-, 4-nitrophenyl ester [9CI] (CA

RN 716327-21-8 CAPLUS
CN 1-Pyrrolidinecarboxylic acid,
3-(3,4-dichlorophenyl)-3-[3-(4-oxo-1-phenyl1,3,8-triazaspiro[4.5]dec-8-yl)propyl]-, ethyl eater (9CI) (CA INDEX NAME)

716327-22-9 CAPLUS
Pyrrolidine,
-chlorophenyl)-1-(2-furanylcarbonyl)-3-[3-(4-oxo-1-phenyl1,3,8-triazaspiro[4.5]dec-8-yl)propyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:745214 CAPLUS
DOCUMENT NUMBER: 132:131772
ITILE: Investigation of SAR requirements of SR 142801
through

AUTHOR (S):

an indexed combinatorial library in solution
Raveglia, Luca F.: Vitali, Mauro: Artico, Marco;
Graziani, Davide: May, Douglas W. P.: Luttmann, Mark
A.: Mena, Renzo: Pifferi, Giorgio: Giardina. Giuseppe
A. M.
Department of Medicinal Chemistry, SmithKline Beecham
S.p.A., Milan, 20021, Italy
European Journal of Medicinal Chemistry (1999).
341[D]: 925-833
CODEN: EJRACAS: ISSN: 0223-5234
Editions Scientifiques et Medicales Elsevier
Journal

CORPORATE SOURCE:

SOURCE:

CODE: EJMCAS: ISSN: 0223-5234

CODE: EJMCAS: ISSN: 0223-5234

Editions Scientifiques et Medicales Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To requiryments of the human neurokinin 3 (hNK-3) receptor antagonist SR

14280f, an indexed combinatorial library was synthesized in solution and

affected on the hNK-3 receptor. SAR considerations drawn from binding

affinity of combinatorial mixts. were confirmed through the synthesis and

biol. evaluation of some individual compds.

IT 256497-28-69

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation): RACT

(Reactent or reagent)

(structure-activity relation requirements of SR 142801 as neurokinin 3

receptor antagonists through indexed combinatorial library in

solution)

RN 256497-28-6 CAPLUS

CN 1-Piperidinecarboxylic acid, 3-(3,4-dichlorophenyl)-3-(3-(4-oxo-1-phenyl1,3,8-triezaspiro(4.5)dec-8-yl)propyl]-, 1,1-dimethylethyl ester (9CI)

REFERENCE COUNT:

THERE ARE 16 CITED REFERENCES AVAILABLE FOR

RECORD, ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2006 ACS ON STN ACCESSION NUMBER: 1998:689192 CAPLUS DOCUMENT NUMBER: 129:330656

DOCUMENT NUMBER: TITLE:

129:330656
Preparation of 1-(3-pyrrolidinylalkyl)-4piperidinecerboxamides as tachykinin antagonists
Burkholder, Timothy P.; Rudlacz, Elizabeth M.; Le
Tieu-binn; Maynard, George D.
Hoechst Marion Roussel Inc., USA
U.S., 93 pp., Cont.-in-part of U.S. 5,635,510.
CODEN: USXXAM INVENTOR(S):

PATENT ASSIGNEE(S): SOURCE:

DOCUMENT TYPE:

FAMILY ACC. NUM. COUNT: PATENT INFORMATION: APPLICATION NO. PATENT NO. KIND DATE DATE 19970211 US 5824690 2A 6403091 US 5635510 PRIGETTY APPLN. INFO.: 19981020 US 1997-798664 ZA 1994-3091

19970603 US 1994-332027 US 1993-58606 19941031 B2 19930506 B2 19940419 US 1994-225371

1026)

US 1994-332027 A2 19941031

OTHER SOURCE(S): MARPAT 129:330656

Title compds. [1: R = G2(CH2)nR2; G1,G2 = CH2 or CO; R1 = (un)substituted Ph, ...naphthy1, pyridy1, etc.; R2 = (un)substituted Ph or -pyridy1; Y1 = CONHRS or CONRER7; R5 = H, alky1, (CH2)qnA6R7, etc.; R6,R7 = alky1; NR6R7 = heterocycly1; Y2 = (un)substituted pheny1(methy1), -pyridy1, -thieny1; Y1Y2 = atoms to complete a ring; Z = (CH2)2-3; n = 0 or 1: q = 2 or 3] were prepared Thus, 3.4-C12C6H3CH2CN was biscondensed with BrCH2CO2Et

were prepared Thus, 3.4-C12Consch2CN was biscondensed with SECRECOZEL

the reduced product cyclized to give, after reduction and N-benzoylation,
]-henzoyl-3-(2-hydroxyethyl)-3-(3,4-dichlorophenyl)pyrrolidine. The
later was treated with MeSOZCI and the product aminated by

T-pholypiperidine-4-carboxamide (preparation given) to give I (GI =

R = C6H3C12-3,4, Y1 = CONH2, Y2 = Ph, Z = CH2CH2). Data for biol.
act ity of I were given.

IT 167261-54-39 167261-55-49

RL: BAC (Bloological activity or effector, except adverse); BSU
(Bloological)

SEM (Bloological) study); PREP (Preparation); THU (Therapeutic use);
biol. (Bloological study); PREP (Preparation); USES (Usea)
['preparation of I-(3-pyrrolidinylalkyl)-4-piperidinecarboxamides as tachykinin antagonists)

RN 107261-54-3 CAPLUS

(02(5)

L4 ANSWER 4 OF 6
ACCESSION NUMBER:
DOCUMENT NUMBER:
1199:504661 CAPLUS
129:245045
Preparation of 3,3-disubstituted piperidines for treating the conditions associated with an excess of tachykinins
INVENTOR(S):
Harrison, Timothy; Swain, Christopher John
Merck Sharp & Dohme Limited, UK
U.S., 17 pp.
CODEN: USXXAM
DOCUMENT TYPE:
Patent

DOCUMENT TYPE:

Patent English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. DATE APPLICATION NO. 19980915 9961018

US 5807865 PRIORITY APPLN. INFO.:

OTHER SOURCE(S); MARPAT 129:245045

11

REFERENCE COUNT:

(03 (A) 6-merhened r.y

The title compds. [I; m=0-2; n=1-3 (with the provise that the sum of m+n=1-4); X=CRIR2; one of Y, Z=0 while the other =R2; Ar=(un) substituted Ph. thienyl, benzothienyl, etc.; R=(un) substituted Ph: RIRZ=(un) substituted Ph:

groups of NRS, etc.; RS = H, C1-4 alkyl, etc.], useful in the treatment

prevention of neuropathy, asthma, osteoarthritis, rheumatoid arthritis or magraine, were prepared Thus, reaction of
5-[3-methanesulfonyloxypropyl]-5[3,4-dichlorophenyl]-1-benzylpiperidin-2-one with 4-acetyl-4phenylpiperidine.HCl in the presence of K2CO3 in DMF afforded 41% I [Y = 0; Z = H2; R = Ph; Ar = 3,4-C12C6H3; n = 1: m = 2; X = CR1R2; R1 = Ph; R2
- Mc(O1). Compds. I are effective at 0.05-10 mg/kg/dsy in the treatment of the conditions associated with an excess of tachykinins.

17 213180-01-9P
RL: BAC (Biological activity or effector, except adverse); BSU
(Biological still activity or effector, except adverse); BSU
(Biological still activity or effector) accept adverse of tachykinins.

(Biclogical study, unclassified); SFN (Synthetic preparation); THU (Therapeutic use); BI(), (Biclogical study); PREP (Preparation); USES (Uses); (preparation of 3,3-disubstituted piperidines for treating the conditions associated with an excess of tachykinins); RN 213180-01-9 CAPLUS CN Piperidine, 1-benroyl-3-(3,4-dichlorophenyl)-3-[3-(4-oxo-1-phenyl-1,3,8-triazaspiro[4.5]dec-8-yl)propyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
CN Pyrrolidine.
3-(3,4-dichlorophenyl)-1-(2,6-dimethoxybenzoyl)-3-+2-(4-oxo-1phenyl-1,3,8-triazaspiro[4.5]dec-8-yl)ethyl]- (9Ct) (CA INDEX NAME)

Porticians (4-oxe-1) -3-(3,4-dichlorophenyl)-3-(2-(4-oxe-1-phenyl-1,3,8-triazaspiro[4.5)dec-8-yl)ethyl)- (9C1) (CA INDEX NAME)

THERE ARE 11 CITED REFERENCES AVAILABLE FOR

(Continued)

RECORD. ALL CITATIONS AVAILABLE IN THE RE

ANSWER 4 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

REFERENCE COUNT:

FORMAT

11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

-1 -5

L4 ANSWEF 5 OF 6 CAPLUS COPYRIGHT 2006 ACS ON STN ACCESSION NUMBER: 1997:375289 CAPLUS DOCUMENT NUMBER: 127:95200
TITLE: SUBSTITUTE: SUBSTITUTE: Substituted pyrrolidin-3-yl-alkyl-piperidines useful

INVENTOR (5):

PATENT ASSIGNER(S):

Substituted by a motifacture and a state of the state of SOUFCE: abandoned

CODEN: USXXAM

DOCUMENT TYPE: LANGUAGE: FAM!LY ACC. NUM. COUNT: PATENT INFORMATION: English

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
· 413-5636410	A	19970603	US 1994-332027	19941031
G12 1124901	A	19960619	CN 1994-192362	19940422
CN 1081635	В	20020327		
ZA 9403091	A	19950112	ZA 1994-3091	19940504
JUE 5648365	A	19970715	US 1995-477167	19950607
561416	A	19990119	US 1997-795576	19970206
US 5824090	A	19981020	US 1997-798664	19970211°
PRINTITY APPLN. INFO .:			US 1993-58606	B2 19930506
			us 1994-225371	82 19940419
		-	US 1994-332027	A3 19941031

MARPAT 127:95200 OTHER SOURCE(S):

$$\begin{array}{c|c}
 & \text{Yl} \\
 & \text{Yl} \\
 & \text{N-Gl-}(CH_2)_n & \text{Ar}^2 \\
 & \text{OMe} \\
 &$$

The invention relates to substituted pyrrolidinyl-3-yl-alkyl-piperidines

ANSWER 5 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued) ANSWER 5 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)
[G. 61 = CH2, CO; m = 2, 3; n = 0, 1; Arl = (un)substituted Ph, naphthyl,
pyridyl, thienyl, or benzo[1,3]dioxan-5-yl, Ar2 = (un)substituted Ph or
pyridyl; Yl = (un)substituted CONH2; Y2 = (un)substituted Ph, naphthyl,
pyridyl, thienyl, or CH2Ph; or YlY2 = atoms to complete certain
Ph-substituted, 5-membered, diazaspiro ring fusions), their

Ph-substituted, 5-membered, diszespiro ring fusions), their stereoisomers,
N-oxides, and pharmaceutically acceptable selts, and processes for prepr. of the same. I are useful for their pharmacol. activities, such as tachykinin entagonism, and esp. substance P and neurokinin A antagonism. Such compds. are indicated for conditions assocd, with neurogenic inflammation and other diseases. For instance, 3-(3,4-dichlorophenyl)-3-(2-hydroxyethyl)pyrrolidine underwent a sequence of amidation with 3,4,5-trimathoxybenzoyl chloride (71%), conversion of the alc. to a methanesulfonate ester (92%), and reaction of the mesylate molety with 4-phenylpiperidine-4-carboxemide-HCl (71%), to give title compd. II. In an assay for modulation of NKA-induced respiratory effects in guinea pigs,

pigs,
II at 10 mg/kg reduced dyspnea to 60% of control.
IT 167261-54-39 167261-55-49
RL: BAC (Biological activity or effector, except adverse): BSU

(Biological study, unclassified): SPN (Synthetic preparation): THU (Therapeutic use): BIOL (Biological study): PREP (Preparation): USES (Uses) (preparation of pyrrolidinylalkylpiperidines as tachykinin

(preparation of pyrroliginysatkyspectation of pyrroliginysatkyspectation of pyrroliginysatkyspectation of pyrroliginys antagonists)
RN 167261-54-3 CAPLUS
CN Pyrrolidine,
3-(3,4-dichlorophenyl)-1-(2,6-dimethoxybenzoyl)-3-(2-(4-oxo-1-phenyl-1,3,8-triazaspiro(4.5)dec-8-yl)ethyl)- (9CI) (CA INDEX NAME)

167261-55-4 CAPLUS Pyrrolidine, 1-benzoyl-3-(3,4-dichlorophenyl)-3-[2-(4-oxo-1-phenyl-1,3,8-triazaapıro[4.5]dec-8-yl]ethyl]- (9C1) (CA INDEX NAME)

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1995:772578 CAPLUS
DOCUMENT NUMBER: 123:198629
TITLE: 9reparation of substituted (pyrrolidin-3ylalkyl)piperidines as tachykinin antagonists
Burkholder, Timothy P.: Le, Tieu-Binh; Kudlacz,
Elizabeth M.; Maynard, George D.
PATENT ASSIGNEE(S): Merrell Dow Pharmaceuticals Inc., USA
POCUMENT TYPE: Patent
LANGUAGE: PIXED2
PAMILY ACC. NUM. COUNT: 3

DOCUMENT TYPE: LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

										APPLICATION NO.										
		9426																		
		W:	AT,	ΑU,	вв,	BG,	BR,	BY,	CA,	CH,	CN	, c	z,	DE,	DK,	ES,	FI.	CB,	HU,	
			JP,	KP,	KR,	KZ,	LK,	LU.	LV,	MG,	MN	, M	w,	NL,	NO,	NZ,	PL,	PT.	RO.	
			RU,	SD,	SE,	SK,	UA,	Uz,	VN											
		RW:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	, 1	E,	IT,	LU,	MC,	ΝL,	FT.	SE.	
				ВJ,																
CA	١	2160	462			AA		1994	1124		CA	199	4 - 2	2160	462		1	9940	422	
CF	١.	2160	462			¢		1998	1215											
		9469									ΑU	199	4-1	6942	6		1	9940	422	
AL	,	6780	23			B2		1997	0515											
E	?	6962	80			A1		1996	0214		EΡ	199	4-	9178	98		1	9940	422	
EF	•	6962 6962	ВО			В1		1997	0924		-		-	٠.	_					
		R:	AT,	BE.	CH,	DE,	DK,	ÉS,	FR,	GB,	GR	, 1	E.	IT,	LI,	LU,	MC,	NL.	PT	
		7408																		
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		3424																		
		1585						1997												
		2110						1998	0216		ES	199	4 -	9178	98					
		1094				A1		2000	10726		ΙL	199	4 -	1094	96			9940		
		9403						1995			ZA	199	4-	3091			1			
		9505						1995			FI	199	5-	5258			1	9951	102	
		1130																		
		9504									ИО	199	5-	4400			1	9951	103	
		3091				В1		2000	1218											
IORIT	۲Y	APP	LN.	INFO	. :						US	199	3-:	5860	6		A I	9930	506	
											US	199	4-	2184	8 3		A 1	9940	328	
											US	199	4-	2253	71		A 1	9940	419	
											wo	199	4-1	U\$44	98		w 1	9940	422	

MARPAT 123:198629 OTHER SOURCE(S):

$$\begin{array}{c|c} Y^1 \\ Y^2 \\ \hline \\ N (CH_2)_m \\ \hline \\ Ar^1 \\ \hline \\ Ar^2 (CH_2)_n Ar^2 \\ \hline \\ 1 \end{array}$$

RN 167262-19-3 CAPLUS
CN Eyrrolidine, 1-benzoyl-3-(3,4-dichlorophenyl)-3-[2-(4-oxo-1,3,8-triamagpire[479]decg8-yl)ethyl]-, (-)- (9CI) (CA INDEX NAME)
Rotation (-).

Rotation (+).

ANSWER 6 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN L4 (Continued)

Title compds. 1 (G1, G2 = CH2, CO; m = 2,3; n = 0,1; Arl. V3 (substituted ryl, (substituted) Ph or https://dx.distributed.ph or https://dx.distributed.ph.co. (distributed) carbony; Arcticocyclyly /1 = (substituted) HNCO, (distributed) carbony; Arheterocyclylcarbonyl; Y1Y2 together with the C to which they are

167261-55-4 CAPLUS Pyrrolidine, 1-benzoyl-3-(3,4-dichlorophenyl)-3-(2-(4-exo-1-phenyl-1,3,8-triazaspiro(4.5]dec-8-yl]ethyl]- 19C1) (CA INDEX NAME)

ANSWER 6 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN

16726)-89-4 CAPLUS
Pyrrolidine, 3-(3,4-dichlorophenyl)-3-[2-(4-fluorophenyl)-2-[4-oxo-3-(phenylmethyl)-1,3,8-triazaspiro[4.5]dec-8-yl]ethyl]-1-(3,4,5-trimethoxybenzoyl)- (9CI) (CA INDEX NAME)

167261-90-7 CAPLUS

RN 16726]-90-7 CAPLUS
CN Pyrrolidine.
1-3-(3,4-dichlorophenyl)-3-[2-[2,4-dioxo-3-(phenylmethyl)-1,3,8triazaspiro[4.5]dec-8-yl]-2-(4-tluorophenyl)ethyl)-1-(3,4,5trimethoxybenzoyl)- (9CI) (CA INDEX NAME)

16726)-91-0 CAPLUS
Pyrrolidine, 3-(3,4-dichlorophenyl)-3-[2-(2,4-dioxo-1,3,8-triazaspic)(4.5)dec-8-yl)-2-(4-fluorophenyl)-thyl)-1-(3,4,5-trimethoxybenzoyl)- (9CI) (CA INDEX NAME)

ANSWER 6 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

167261-86-1 CAPLUS
Pyrrolidine,
4-dichlorophenyl)-3-[2-(4-oxo-1,3,8-triazaspiro[4.5]dec-8-yl)ethyl]-1-(3,4,5-trimethoxybenzoyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{OMe} \\ \text{MeO} \\ \\ \text{C} \\ \text{C} \\ \text{N} \\ \end{array}$$

RN 167261-87-2 CAPLUS CN Pyrrolidine, 3-(3,4-dichlorophenyl)-3-[2-(4-oxo-1,3,8-triazaspiro[4.5]dec-1-en-8-yl)ethyl]-1-(3,4,5-trimethoxybenzoyl)- (9CI) (CA INDEX NAME)

167261-88-3 CAPLUS
Pyrrolidine, 3-(3,4-dichlorophenyl)-3-[2-(4-fluorophenyl)-2-(4-oxo-1,3,8-triazaspird,4.5|dec-8-yl)ethyl|-1-(3,4,5-trimethoxybenzoyl)- (9CI) (CA INDEX NAME)

L4 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 167262-05-7 CAPLUS
CN Pyrrolidine,
3-(3,4-dichlorophenyl)-1-(2,6-dimethoxybenzoyl)-3-[2-(4-oxo-1-phenyl-1,3,8-triazaspiro[4.5]dec-8-yl]ethyl]-, (+)- (9CI) (CA INDEX NAME)

Rotation (+).

RN 167262-06-8 CAPLUS
CN Pycrolidine,
3-(3,4-dichlorophenyl)-1-(2,6-dimethoxybenzoyl)-3-(2-(4-oxo-1-phenyl-1,3,8-triazaspiro(4,5)dec-8-yl)ethyl]-, (-)- (9CI) (CA INDEX

Rotation (-).